Quantization and Corrections of Adiabatic Particle Transport in a Periodic Ratchet Potential

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Abstract

We study the transport of an overdamped particle adiabatically driven by an asymmetric potential which is periodic in both space and time. We develop an adiabatic perturbation theory after transforming the Fokker-Planck equation into a time-dependent hermitian problem, and reveal an analogy with quantum adiabatic particle transport. An analytical expression is obtained for the ensemble average of the particle velocity in terms of the Berry phase of the Bloch states. Its time average is shown to be quantized as a Chern number in the deterministic or tight-binding limit, with exponentially small corrections. In the opposite limit, where the thermal energy dominates the ratchet potential, a formula for the average velocity is also obtained, showing a second order dependence on the potential.

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The so-called ratchet models have attracted much interest in recent years [1–3]. In a typical ratchet model, a driving force with time-correlated fluctuation, in addition to a random force, is exerted on an overdamped particle. A macroscopic flow develops if the parity symmetry is broken in the driving potential. This behavior is in striking contrast to the equilibrium situation in which the second law of thermodynamics forbids a non-vanishing macroscopic flow, irrespective of the microscopic details [4]. Here we consider an adiabatic ratchet potential with both spatial and temporal periodicities, which has received some attention recently [5,6]. We take an analytical approach by transforming the Fokker-Planck equation into a time-dependent hermitian problem. The ensemble average of the particle velocity is calculated by using the standard adiabatic perturbation theory, whose validity condition is also explicitly specified for the present system. The particle transport in a time cycle is found in terms of the Berry phase of the Bloch waves. In the deterministic or tight-binding limit, in which the potential dominates the thermal energy, the particle transport is shown to be quantized as a Chern number [7], consistent with the previous numerical result [5], and in analogy with quantum adiabatic particle transport first studied by Thouless and Niu [8–10]. The correction to the quantization is found to be exponentially small based on an analysis using the Wannier functions. We also elaborate the opposite limiting case, where the thermal energy dominates the potential.

Consider an overdamped particle moving in one-dimension, subject to a driving force $F(x,t) = -\partial_x V(x,t)$ and a random force $\nu(t)$. It obeys a Langevin equation,

$$\gamma \frac{dx}{dt} = \frac{1}{\mu} F(x,t) + \nu(t),$$

where γ is the friction constant and μ is the mass. We assume that $\nu(t)$ is of zero average and δ-correlated, i.e. $\langle \nu(t)\nu(t')\rangle = 2(\gamma k_B T/\mu)\delta(t-t')$, where k_B is the Boltzmann constant, T is the temperature, and $\langle \cdots \rangle$ denotes the ensemble average. The potential $V(x,t)$ is periodic in both space and time, with periods a and τ respectively. Furthermore, the potential is assumed to be asymmetric, i.e. $V(x) \neq V(-x)$, as shown in Fig. 1.

The corresponding Fokker-Planck equation for the probability density $\rho(x,t)$ is

$$-\partial_t \rho(x,t) = D\mathcal{O}\rho(x,t), \tag{1}$$

where $D = k_B T/\mu\gamma$ is the diffusion constant, and $\mathcal{O} = -\partial_x^2 + \partial_x \cdot F/k_B T$. The Fokker-Planck equation (1) can also be written as a continuity equation $\partial_t \rho + \partial_x j = 0$, where the probability current is $j(x,t) \equiv D\hat{j}\rho(x,t)$, with $\hat{j} = -\partial_x + F/k_B T$.

The operator $\mathcal{O}$ is non-hermitian, but there is a similarity transformation [11] leading to a hermitian operator, to be called the effective hamiltonian,

$$\mathcal{H} = e^{\Gamma}\mathcal{O}e^{-\Gamma} = \hat{p}^2 + U, \tag{2}$$

where $\Gamma = V/2k_B T$ is the potential normalized by the thermal energy, $U = (\partial_x \Gamma)^2 - \partial_x^2 \Gamma$ is the effective potential, and $\hat{p} = -i\partial_x$. Note that $\mathcal{H}$ has the dimension of inverse length squared. Since $\mathcal{H}$ is hermitian, its eigenfunctions comprise a complete orthonormal basis. These are the Bloch waves, ψ_{nk}, owing to the periodicity of the potential, where n is the discrete band index, and k is the Bloch vector. It is also interesting and useful to note that the ground state eigenvalue is zero, and the wave function can be explicitly found as

$$\psi_0 = \frac{1}{\sqrt{Z}} e^{-\Gamma},$$

where $Z = \int e^{-2\Gamma} dx$ is a normalization factor ensuring $\langle\psi_0|\psi_0\rangle = \int \psi_0(x)^*\psi_0(x)dx = 1$.

The Fokker-Planck equation is then transformed into

$$-\partial_t\psi(x,t) = (D\mathcal{H} - \partial_t\Gamma - \partial_t \ln\sqrt{Z})\psi(x,t), \tag{3}$$

where $\psi = \rho e^{\Gamma}\sqrt{Z}$ is the transformed variable for the probability density, and the factor $\sqrt{Z}$ is added for convenience. If $\psi = \psi_0$, then the probability density is the stationary Boltzmann distribution $\rho = e^{-2\Gamma}/Z$, giving $j = 0$. If V were time-independent, the above equation would reduce to $-\partial_t\psi = D\mathcal{H}\psi$, whose ground state solution $\psi = \psi_0$ corresponds to the equilibrium state.

The wave function ψ is generally a superposition of different Bloch states. However, only those with k=0 are important if we are only interested in the ensemble average of the particle velocity $\langle\frac{dx}{dt}\rangle$. This is equal to the spatial integral of the probability current,

$$J(t) = D\int \hat{j}\rho dx = D\int \psi_0(-\partial_x - \partial_x\Gamma)\psi dx = -2D\int \psi_0\partial_x\psi(x,t)dx, \tag{4}$$

where, in the expansion of $\psi(x,t)$, only $\psi_{nk}(x,t)$ with $k = 0$ contribute. This result does not require the necessity of adiabaticity.

We now apply the adiabatic perturbation theory [12], supposing that the ratchet potential changes slowly. We first make the expansion

$$\psi(x,t) = \sum_n c_n(t)\psi_n(x,t)e^{-D\int_0^t E_0(t')dt'}, \tag{5}$$

where $k = 0$ is assumed in light of the discussions above. For clarity, we have retained E_0 although it is zero. The coefficient for the ground state is constrained to $c_0(t) \equiv 1$ as imposed by the normalization of the density $\rho(x,t)$. The coefficients for the higher bands satisfy

$$D(E_0 - E_n)c_n + \sum_{n'} c_{n'}\langle\psi_n|\partial_t\Gamma + \partial_t \ln\sqrt{Z} - \partial_t|\psi_{n'}\rangle = \partial_t c_n. \tag{6}$$

The terms in the summation are small if the potential changes slowly and if we choose the Bloch waves with $k = 0$ to be real such that $< \psi_n|\partial_t|\psi_n >= 0$. We also assume that the system is initially in the ground state (stationary state). Thus we can ignore all but the $n' = 0$ term in the summation, obtaining, to first order in the rate of change of the potential,

$$c_{n\neq 0}(t) = \frac{2\langle\psi_n|\partial_t\psi_0\rangle}{D[E_0(t) - E_n(t)]}, \tag{7}$$

where we have used the fact that $(\partial_t\Gamma + \partial_t \ln\sqrt{Z})\psi_0 = -\partial_t\psi_0$. The smallness of c_n for $n > 0$ means that the system remains close to quasi-static equilibrium with the instantaneous ratchet potential. If the system has initial excitations in the higher bands, one can show that they decay away exponentially at a rate of $D(E_n - E_0)$ and become negligible after a transient period.

Quantitatively, the adiabatic condition is satisfied if the potential changes at a rate much smaller than D times the eigenvalue gap, $\frac{1}{\tau} \ll D(E_1 - E_0)$. We now make an order of magnitude estimate of this gap. We assume that the amplitude of variation in the force is

F_0, yielding the variation for Γ as $\Gamma_0 = F_0 a/2k_B T$. In the kinetic regime where $\Gamma_0 << 1$, the gap at $k = 0$ is about $(2\pi/a)^2$. The adiabatic condition is just $\tau \gg \tau_D$, where $\tau_D = a^2/D$ is the diffusion time over one wavelength of the ratchet. In the tight-binding or deterministic regime, where $\Gamma_0 >> 1$, the Bloch bands may be viewed as derived from the levels in the deep potential wells. A peculiar thing to notice is that the effective potential U typically contains a double well structure in each wavelength of the ratchet, even if the ratchet potential has one well in each period. The reason is that the dominant term $(\partial_x \Gamma)^2$ in U has only half of wavelength of the ratchet, and thus must contain two wells in each wavelength of the ratchet. These two wells are made inequivalent by the weaker term, $-\partial_x^2 \Gamma$, which has the full periodicity of the ratchet. The band gap can thus be estimated by the level difference between the two wells, and is given by the amplitude of variation of the weaker term Γ_0/a^2. The adiabatic condition in this case is $\tau \gg \tau_D/\Gamma_0$, which is more easily satisfied than the kinetic regime because of the large Γ_0 in the tight-binding regime.

The average velocity induced by the adiabatic movement of the ratchet can then be obtained from (4), (5) and (7) as

$$J(t) = -4 \sum_{n \neq 0} \frac{\langle \psi_0 | \partial_x \psi_n \rangle \langle \psi_n | \partial_t \psi_0 \rangle}{E_0 - E_n}, \tag{8}$$

This current is independent of the diffusion constant D, because all the eigenstates and eigenvalues of the effective Hamiltonian are independent of D. This signifies that the adiabatic flow is a geometric effect: it only depends on how the ratchet potential evolves in time, and is independent of the mobility of the particles. The only role of the diffusion constant is to set the time scale for the validity of the adiabatic approximation. The reader is also reminded that the distinction between the tight-binding and kinetic regimes, in which the adiabatic flow will be shown to have very different behaviors, also has nothing to do with D.

In the following, we make a further connection to the Berry phase, and show when the adiabatic current may be quantized. We can write $J(t) = \mathcal{J}(k = 0, t)$, with

$$\mathcal{J}(k, t) = -2 \sum_{n \neq 0} \left[\frac{\langle \psi_{0k} | \partial_x \psi_{nk} \rangle \langle \psi_{nk} | \partial_t \psi_{0k} \rangle}{E_{0k} - E_{nk}} + \frac{\langle \partial_t \psi_{0k} | \psi_{nk} \rangle \langle \partial_x \psi_{nk} | \psi_{0k} \rangle}{E_{0k} - E_{nk}} \right]. \tag{9}$$

This can be rewritten in terms of the periodic amplitude $u_{nk}(x, t)$ of the Bloch waves, and turned into a form involving the lowest band only

$$\mathcal{J}(k, t) = \frac{1}{i} \left[\langle \partial_k u_{0k} | \partial_t u_{0k} \rangle - \langle \partial_t u_{0k} | \partial_k u_{0k} \rangle \right], \tag{10}$$

following the method used in deriving the quantum adiabatic particle transport [8,9]. This is known as the Berry curvature of the Bloch state in the parameter space of k and t. The time average of $J(t)$ over a time cycle of the ratchet is therefore

$$\overline{J(t)} = \frac{1}{i\tau} \int_0^\tau dt \left[\langle \partial_k u_{0k} | \partial_t u_{0k} \rangle - \langle \partial_t u_{0k} | \partial_k u_{0k} \rangle \right]_{k=0} = -\frac{1}{\tau} \partial_k \theta(k)_{k=0}, \tag{11}$$

where $\theta(k) = i \int dt \langle u_{0k} | \partial_t u_{0k} \rangle$ is the Berry phase for a given k. In obtaining the last expression in the above equation, we assumed a phase gauge such that the wave function is

periodic in time, which is possible because the eigenstate must come back to itself in a time cycle of the potential apart from a phase factor.

In the tight-binding or deterministic limit, the quantity $\mathcal{J}(k,t)$ is insensitive to k, as can be seen in (9), which can be be written as

$$\mathcal{J}(k,t) = 2\left[\langle\partial_x\psi_{0k}|\frac{1}{E_{0k}-\mathcal{H}}|\partial_t\psi_{0k}\rangle + \langle\partial_t\psi_{0k}|\frac{1}{E_{0k}-\mathcal{H}}|\partial_x\psi_{0k}\rangle\right]. \tag{12}$$

We may thus replace the $k=0$ expression in (11) by an average over k, yielding

$$\overline{J(t)} = \frac{a}{2\pi i\tau}\int_0^{2\pi/a} dk \int_0^{\tau} dt\,[\langle\partial_k u_{0k}|\partial_t u_{0k}\rangle - \langle\partial_t u_{0k}|\partial_k u_{0k}\rangle]\,. \tag{13}$$

This is a closed surface integral of the Berry curvature, and can only take quantized values, i.e.

$$\overline{J(t)} = N\frac{a}{\tau},$$

where N is an integer called Chern number.

Corrections to this exact quantization, which arise in our replacing the k=0 expression by an average over k, can be shown to be exponentially small in Γ_0. Consider first the somewhat trivial example of a sliding potential, $V(x-vt)$, which is in general not a ratchet. The position and time dependence of the Bloch states must be through the combination $x-vt$. We can thus replace ∂_t by $-v\partial_x$, turning (8) into an expression related to the "effective mass" of a band [10]. The result is that the average particle current can be written in the form $v[1-2^{-1}\partial^2 E_{0k}/\partial k^2|_{k=0}]$. The first term is just the quantization with $N=1$, which means that the particle follows the potential, while the second term is exponentially small in Γ_0 because the band width is so in the tight-binding limit.

To establish the exponential smallness of the correction to quantization for the general case of the tight-binding regime, we introduce the the Wannier functions $\phi_n(x-la) = \frac{a}{2\pi}\int dk e^{-ikla}\psi_{nk}$, which are known to be exponentially localized and form an orthonormal basis for each band. We may rewrite (10), with $k=0$, as

$$J(t) = \partial_t\langle x\rangle + a\sum_l l\langle\phi_0(x,t)|\partial_t\phi_0(x-la,t)\rangle, \tag{14}$$

where $\langle x\rangle \equiv \langle\phi_0(x,t)|x|\phi_0(x,t)\rangle$ is the center position of the Wannier function [10]. In deriving the above result, it is useful to recall the inverse relation $\psi_{nk}(x,t) = \frac{1}{\sqrt{M}}\sum_l e^{ikla}\phi_n(x-la,t)$ between the Bloch and Wannier functions, where M is the number of cells in the system. Therefore

$$\overline{J(t)} = \frac{1}{\tau}(\langle x\rangle|_{t=\tau} - \langle x\rangle|_{t=0}) + \frac{a}{\tau}\sum_l l\int_0^{\tau} dt\langle\phi_0(x,t)|\partial_t\phi_0(x-la,t)\rangle. \tag{15}$$

$\langle x\rangle$ can only change by an integer multiple of the lattice constant in a time period, so the first term in (15) is nothing but the quantization Na/τ. The second term gives a correction to this quantization. Contribution from $l=0$ term is automatically zero. In the tight-binding limit, these Wannier functions decay exponentially away from the bottom of each well, so the leading term in the correction comes from the nearest-neighbor term $l=1$. Therefore, the

correction is proportional to the overlap between the nearest-neighboring Wannier functions, which is exponentially small in Γ_0.

On the other hand, beyond the tight-binding or deterministic limit, the quantization is destroyed. We now consider the opposite limit, the kinetic regime where $\Gamma_0 << 1$. We can make a perturbative expansion the Bloch function in terms of the plane waves, $\psi_{0k} = \sum_m c_m(k)e^{i(k+m2\pi/a)x}$, where $c_0(k) = 1$ and $c_m = U_m/[k^2 - (k+2\pi m/a]^2)$ for $m \neq 0$, with $U_m = \int U(x,t)e^{-im2\pi x/a}dx$ being the Fourier coefficient of the effective potential. Because we are interested in the neighborhood of $k = 0$, no degeneracy needs to be considered. The average velocity is calculated as $J(t) = \frac{2}{i(2\pi/a)^5}(U_{-1}\partial_t U_1 - U_1\partial_t U_{-1}) = \frac{4}{(2\pi/a)^5}|U_1|^2\partial_t\theta_1$, where θ_1 is the phase of U_1, and the higher order terms with $|m| > 1$ have been dropped. Therefore, $J(t)$ is proportional to the absolute square of the potential and to the rate of phase change in the potential.

To summarize, we have considered a ratchet model in which an overdamped particle is adiabatically driven by an asymmetric potential which varies periodically both in space and in time. The problem is treated by transforming the time-dependent Fokker-Planck operator to a time-dependent hermitian operator. The spatial periodicity validates the use of adiabatic theorem, which allows us to develop an adiabatic perturbation theory based on the instantaneous eigenfunctions of the hermitian operator. There are two limiting regimes, determined only by which of the potential energy and the thermal energy dominates. For each of these limiting regimes, we have discussed the adiabatic condition, for which the diffusion constant D sets the time scale. We then calculate the ensemble average of the particle velocity, which is independent of D. The necessity of parity symmetry breaking is reflected in that otherwise the relevant integrals vanish. An analytical expression of the average velocity is obtained in terms of the Berry curvature and Berry phase of the Bloch states. In the deterministic or tight-binding limit, i.e. when the potential dominates the thermal energy, the time average of the average velocity is found to be quantized as a Chern number, with exponentially small corrections. This analytical result confirms and extends a previous numerical observation, and discloses the analogy with the problem of quantum adiabatic transport. On the other hand it provides, in a classical statistical system, a physical example of the first Chern characteristic class, which has been important in gauge field theory [13] and in quantum condensed matter physics [8–10,14]. We have also discussed the kinetic limit, in which the thermal energy dominates the potential. Throughout our work, we have emphasized the effects of geometry and phases.

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FIGURES

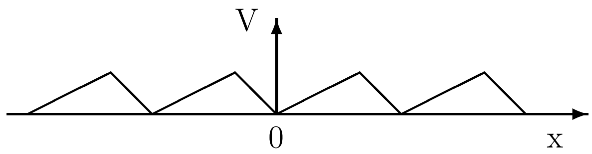

FIG. 1. An illustration of a ratchet potential $V(x,t)$ which is periodic, but asymmetric, in space. In our consideration, it is also periodic in time.

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